Direct Simulation Monte Carlo Benchmarking and Code Comparison

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A wide variety of applications require a core capability to model fluid flow on the subcontinuum scale. Direct Simulation Monte Carlo (DSMC) is the standard methodology used to model these types of flows.

The purpose of our project is to apply a series of available DSMC codes to two classes of problems. The first set comprises simple benchmark problems that contain either known or analytical solutions, which provides us confidence in our ability to use the codes effectively. The second set contains problems that are pertinent to LLNL applications, which allows us to determine which code contains the best capabilities to handle a given type of problem. Three suites of freely obtained codes were used: DS2V/DS3V; the DSMC Analysis Code (DAC); and MONACO2d/3d.

To supplement our study, we created fluid mesh generation tools to allow for efficient implementation of the codes. In addition, we performed traditional continuum CFD analysis of several of the benchmark problems at noncontinuum flow conditions. The results of this analysis demonstrated the loss of convergence ability in the CFD solver as the flow conditions deviate from the continuum limit.

Finally, we interviewed known leaders in the DSMC field to obtain their opinions regarding the usage of the aforementioned codes for certain types of problems.

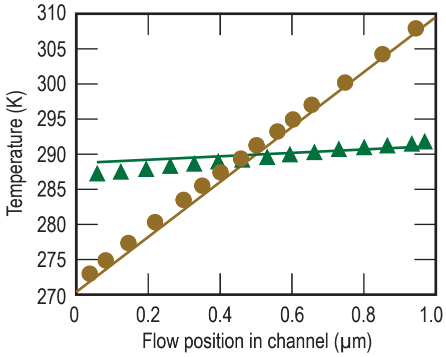

Figure 1. DSMC (lines) and analytical (markers) solutions to the steady-state temperature field of Ar in a 1-μm channel for a Knudsen number of 0.01 (brown) and 10 (green), where the wall temperatures are 270 K and 310 K.

Project Goals

The major goal of our study is to implement the codes on both classes of problems mentioned above in order to assess the accuracy of various code features. Systems ranged from internal flow problems such as a simple comparison of a temperature gradient in a microchannel using DSMC to an analytical temperature slip model (Fig. 1), or a model of an experimental chemical vapor deposition apparatus compared to experimental results (Fig. 2).

We also modeled chemically reacting external re-entry flows (Mach number > 18) for a cylinder (Fig. 3) and a sphere (Fig. 4).

Relevance to LLNL Mission

Systems containing subcontinuum fluids are seen in a wide variety of applications around the Laboratory, which generally feature very small length scales or low density (rarefied) gas conditions. Examples of the former group of systems include flow near sensors or inside microchannels, while the latter group includes microfabrication processes and vehicle re-entry scenarios. One of the LLNL-specific benchmarks we applied the codes to is a magnetron sputtering chamber used for growing films on large scale adaptive optics, which also has relevance to the microfabrication cluster tool and NIF target capsule manufacturing.

FY2007 Accomplishments and Results

We successfully modeled six general problems and three LLNL-related problems using the codes DAC and DS2V. We also examined the use of

DS3V in the magnetron sputtering chamber analysis, and we applied the MONACO2d code for use in a re-entry chemistry sensitivity study. We obtained good agreement with analytical solutions for the classic Fourier problem (Fig. 1) and flow in a microchannel. Good agreement was also achieved when compared to experimental and modified continuum simulations of the CVD chamber shown in Fig. 2. We also showed good code agreement between DAC and DS2V in a variety of external flow problems. All of our findings are available in a report that provides guidance on the advantages and disadvantages of using each DSMC code, when a continuum code is proper for a given type of problem, and which DSMC code options are the most appropriate for a given system.

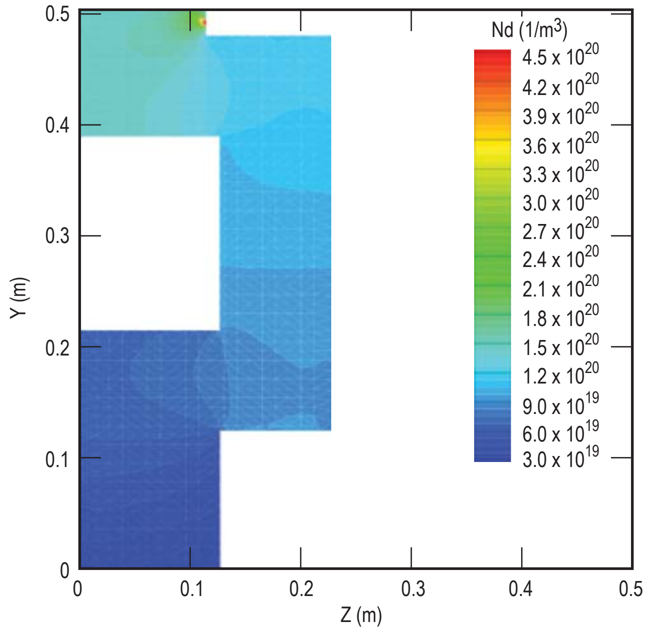

Figure 2. Simulation of Ar number density in a chemical vapor deposition chamber following the study of Singh *et al.*

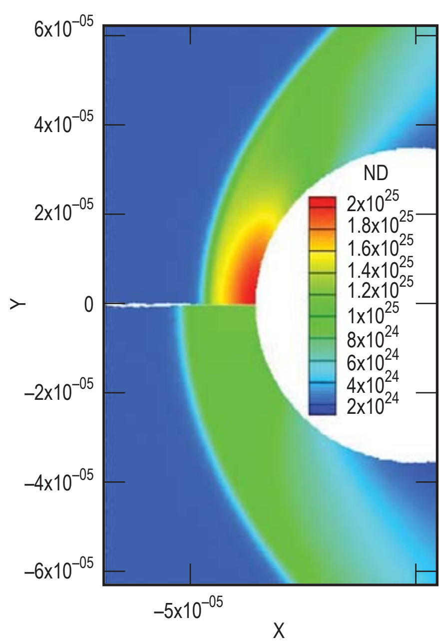

Figure 3. Number density for air impinging upon a cylinder at Mach 18. The upper and lower plots show results for reacting and nonreacting flow, respectively.

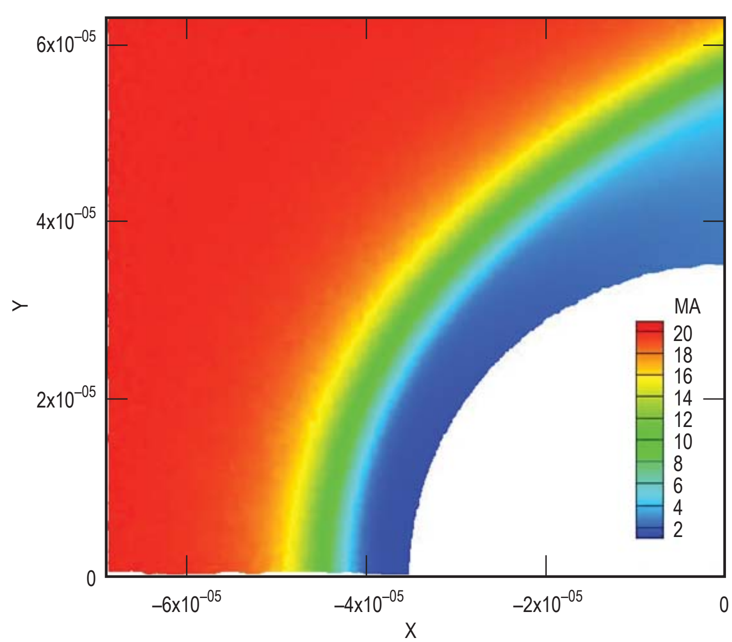

Figure 4. The simulated local Mach number for reacting airflow at 5901.38 m/s, 216.7 K, and 1.8487×10^{24} m^{-3} around a 0.07-mm-diameter sphere.

Related References

1. Davis, D. H., "Monte Carlo Calculation of Molecular Flow Rates Through a Cylindrical Elbow and Pipes of Other Shapes," *J. Appl. Phys.*, **31,** 7, pp. 1169-1176, 1960.
2. LeBeau, G. J., and F. E. Lumpkin, "Application Highlights of the DSMC Analysis Code (DAC) Software for Simulating Rarefied Flows," *Comp. Meth. Appl. Mech. Eng.*, **191,** 6-7, pp. 595-609, 2001.
3. Dietrich, S., and I. D. Boyd, "Scalar and Parallel Optimized Implementation of the Direct Simulation Monte Carlo Method," *J. Comp. Phys.*, **126,** pp. 328-342, 1996.
4. Singh, V., B. Berney, and A. Krishnan, "Designing Low Pressure Systems With Continuum Models," J. *Vac. Sci. Technol. A*, **14,** 3, pp. 1252-1257, 1996.
5. McNenly, M. J., A. P. Wemhoff, and H. Hsieh, "Sensitivity of a DSMC Solution to the Thermochemistry Model for Non-Equilibrium Reentry Flows," *DSMC Theory, Methods, and Applications Conference*, Santa Fe, New Mexico, Sept. 30 – Oct. 3, 2007.